X-ray Optics Considerations for Enhancing Beamline Performance

The quality of X-ray optics has an enormous impact on the performance of synchrotron radiation (SR) beamlines in terms of resolution, data collection rates, and ease of operation. There are many different optical components and all affect the productivity of a beamline. Some elements might seem innocuous like windows, filters, and slit systems, but in practice can have a significant impact on beamline performance and thus require careful consideration. To make the point, many beamlines currently operate with many windows and if the window material, or even its necessity, is not considered carefully, one may suffer significant and unnecessary cumulative losses that deteriorate beamline performance. These cumulative losses can be surprisingly large and one should consider limiting the number of windows wherever possible. Beryllium is the most common material for X-ray windows and even with the highest purity of beryllium that is commercially available (99.8% pure), the absorption due to the impurities is equal to the absorption due to the beryllium at approximately 18 keV. For lower energies, the absorption due to the impurities will dominate – at 10 keV, 2.3 mm will result in a factor of two loss. For lower grades of beryllium, the situation is significantly worse. For many beamlines, significant gains may be made simply by improving, or better, removing windows even if it comes at additional cost.

Apart from windows, filters, and slit systems, 90% of the remaining SR beamline optics involve monochromators and focusing elements. Other optics such as X-ray polarizers, phase retarders, flat mirrors, beam-expanders, beam-splitters, interferometers, et cetera are also needed for certain measurements, but may be considered specialty optics that have seen only sporadic development over the years. Monochromatization and focusing have experienced significant advances in the past 15 years and it is worth outlining some of the current directions of research that are affecting available resolutions and efficiencies. In the next five years, there is an opportunity for further advancement in these areas if appropriate resources for doing so are allocated now.

Monochromatization

Currently, cryogenically-cooled silicon and water-cooled diamond monochromators are performing reasonably well at energies where most measurements are performed. Amidst possible source upgrades, the question of continued good performance needs to be examined. Heat-load issues remain an uncertain area without knowing the degree to which power loads may increase due to the possibility of higher stored current and/or improved insertion devices that produce greater radiative power. Well-engineered versions of the two designs above should perform well for modest increases in power load.

Primary monochromators typically produce energy resolutions ($E/\Delta E$) of 10^4. To achieve higher resolutions, a secondary monochromator is needed. In the 5-40 keV energy range, resolutions are readily achievable that can produce bandwidths down to 10 meV with good spectral efficiency (50%-90%). Producing 1 meV bandwidths can be done with approximately 50% spectral efficiency using cryogenic technology. Producing a 0.1 meV bandwidth has been demonstrated, but building an instrument suitable for a user community would require development. Provided with adequate resources, such an instrument can be produced within five years.

For X-ray energies 40-80 keV, there has been little development to date with regard to high resolution. If high energy-resolution were needed, moderate development should be able to realize energy bandwidths as low as 5 meV with spectral efficiencies of 50%. This level of spectral filtering at high energies has yet to be demonstrated, but would be a reasonable goal given adequate resources.

Energy analysis of large, divergent, X-ray beams is generally needed for spectroscopy to analyze the energy spectrum of scattered radiation. Currently, near-back-reflection analyzers can achieve energy acceptances around 1 meV, but suffer from low efficiency. The low efficiency is not intrinsic, but is related to the fabrication process. With allocation of appropriate resources, this could be improved significantly by developing a reliable procedure to manufacture highly efficient analyzers. As for improving the energy resolution of analyzers, there is currently no practical way to efficiently filter a large, divergent, X-ray beam with an energy bandwidth in the range of 0.1 to 0.5 meV.

Focusing

There has been significant developments in focusing in the last 10-15 years. As a result, there are many focusing techniques and each has its respective advantages. Kirkpatrick-Baez (K-B) mirror systems, zone plates, and refractive lenses are the leading focusing technologies that are currently experiencing the most interest. All three of these technologies have demonstrated focal spot sizes that are well below 100 nm. Resolutions for all three device types are limited currently by fabrication difficulties that may be overcome in the near future.

K-B mirror systems are very versatile with a large parameter space of acceptable efficiency versus focal spot size. One can achieve few micron focal spots with full beam acceptance and good overall efficiency. Focal spot sizes as small as 25 nm have been reported. In the near term, focal spot sizes may be decreased further (say to 10 nm). If one may forgo the achromatic nature of total external reflection, it is possible to fabricate the reflecting mirrors as multi-layers and use a multi-layer Bragg reflection to increase the incident angle, which reduces the beam footprint and would allow the size of the optic to be reduced. K-B mirror systems should be considered for focusing x-rays with energies below say 70 keV. This approximate upper limit is due primarily to the low critical angle for total external reflection or low reflectivity in the case of a multilayer. Their advantages include good efficiency over a wide energy range and an achromatic response when using total external reflection.

Zone plates currently achieve few tens-of-nanometers sized focal spots. Again the limiting issue is related to fabrication. A number of alternative methods of fabrication and operation have been reported and steady progress may allow one to achieve 5-10 nm focal spots in the not so distant future. Zone plates should be considered for energies below 30 keV. At higher energies the thickness of the zone plate has to become large to achieve the requisite phase shift and the zone width of the outermost zone determines the focal spot size. This leads to aspect ratios and geometrical tolerances that are difficult to achieve without sacrificing overall efficiency. Their advantages include relatively good efficiency for sub-micron focusing, an in-line geometry, relatively easy operation, and relatively low cost.

Refractive lenses have also seen significant advances in recent years and have demonstrated focal spot sizes that are as small as a few tens of nanometers. Employing evermore sophisticated fabrication techniques may allow even smaller focal spot sizes in the future. They are usable over a very wide energy range; from 6 keV at the low end to many hundreds of keV at the high end. Their advantages include a wide range of focal spot sizes, an in-line geometry, relatively easy operation, and relatively low cost.

It is difficult to compare the three main focusing techniques without having a specific application in mind. This is because the optimal choice depends on many things such as energy, energy range, cost, beamline layout, needed working distances, and the inevitable trade-off between focal spot size and overall efficiency. With regard to overall efficiency, focusing to 30nm can be done today, but any technique for doing so results in overall efficiencies that are well below 1%. In the next five years, it may be possible to reduce focal spot sizes to 10nm, or even smaller. Perhaps a question more relevant to the majority of beamlines would be how much can efficiencies be improved. As this would make nano-focusing more accessible to a wider range of X-ray scattering techniques, as well as, improve data collection rates for existing techniques. Improving efficiencies will require greater control over the optic fabrication process and perhaps modifying source properties, but the possibility of employing multiple focusing systems to achieve larger acceptance of the SR phase space needs to be explored.

Shaped mirrors that produce 2-dimensional focusing in a single reflection are employed at many beamlines for full-beam focusing. The manufacturing and bending of such mirrors requires figure error tolerances that are exceedingly difficult to achieve. Alternative focusing schemes should be at least considered. K-B mirror systems tackle the problem of 2-dimensional focusing in two steps. As a result, the tolerances for fabrication and operation are more relaxed. This makes small focal spots more readily attainable with greater efficiency resulting in superior performance even though there is an additional reflection. Also, refractive lens technology is improving steadily and one should consider this for full-beam focusing. For beamline applications that use different energies, this may require multiple refractive lens configurations to accommodate their chromatic behavior.